

Asymptotic Positivity of Hurwitz Product Traces

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Abstract

Consider the polynomial $\text{tr}(A + tB)^m$ in t for positive hermitian matrices A and B with $m \in \mathbb{N}$. The Bessis-Moussa-Villani conjecture (in the equivalent form of Lieb and Seiringer) states that this polynomial has nonnegative coefficients only. We prove that they are at least asymptotically positive, for the nontrivial case of $AB \neq \mathbf{0}$. More precisely, we show that the k -th coefficient is positive for all integer $m \geq m_0$, where m_0 depends on A , B and k .

1 Introduction

Some 30 years ago, Bessis, Moussa and Villani (BMV) conjectured [1]¹ that for any hermitian $n \times n$ matrices A and B , the function

$$\mu(t) := \text{tr} \exp(A - tB)$$

with $t \in \mathbb{R}$ is the Laplace transform of a positive measure on $[0, \infty)$, provided B is positive². Lieb and Seiringer [10] proved that this statement is equivalent to the assertion that, for positive integers m and positive hermitian A and B , the polynomial

$$\text{tr}(A + tB)^m = \sum_k \text{tr} S_{m,k}(A, B) t^k$$

has nonnegative coefficients only. Here, the Hurwitz product $S_{m,k}$ [6] equals the sum of all words in A and B , containing $m - k$ letters A and k letters B . Although the conjecture is widely expected to be true, there are, by now, only partial results confirming it. Of course, it is true in the obvious cases of commuting A and B , for $n = 1$ and for $k \leq 2$. For $n = 2$, the statement follows since there is a common basis where A and B have nonnegative entries only [10]. Beyond that, positive results have been obtained for lower m ; at present, the conjecture is proven for $m \leq 13$ [8, 6]. This relied on two main ideas: First, generally, if the

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¹Originally, in [1], a stronger conjecture has been stated: For any bounded-from-below self-adjoint operators A and B and any eigenvector φ of B , the function $\langle \varphi, e^{-(A+tB)} \varphi \rangle$ is the Laplace transform of a positive measure μ whose support is contained in the convex hull of the spectrum of B . This conjecture, however, turned out to be wrong as seen by Froissart (see the notes added in proof in [1]; alternatively, see the example given in [4]). Then, BMV conjectured that, nevertheless, the statement remains valid for the trace.

²Positivity of a hermitian matrix B means that $\langle x, Bx \rangle \geq 0$ for all $x \in \mathbb{C}^n$. In particular, $\mathbf{0}$ is positive.

conjecture is given for some (m, k) , then it holds for any (m', k') with $m' \leq m$, $k' \leq k$ and $m' - k' \leq m - k$ [6]. Second, more specifically, Hägele [5] proposed to write $S_{m,k}(A, B)$ —up to some cyclic permutations—as a sum of positive terms. Although not possible for $(6, 3)$ and several other cases [9], he was able to find such a decomposition for $(7, 3)$, implying the BMV conjecture for $m \leq 7$. More refined methods [8] using computer algebra established the cases $(14, 4)$ and $(14, 6)$, implying the conjecture for $m \leq 13$. Recently, it has been shown that the conjecture is always true for $k = 4$ [3]. Other results show that one may restrict oneself to the case of singular matrices A and B when proving the conjecture inductively [6]. Although the BMV conjecture is still open, it is known that the untraced coefficients $S_{m,k}(A, B)$ need not be positive. The easiest example is $S_{6,3}(A, B)$ for appropriate A and B ; here, some single words may even have negative trace [7].

In the present paper we study a different side of the problem. Shifting the focus from (computer) algebra back to analysis, we are going to investigate the behaviour of the terms $\text{tr } S_{m,k}(A, B)$ for large instead of small m . Our main result is³

Theorem 1.1 Let A and B be positive hermitian $n \times n$ matrices and $k \in \mathbb{N}$. Then there is some $m_0 \in \mathbb{N}$, such that:

$$\begin{aligned} AB = \mathbf{0} &\implies \text{tr } S_{m,k}(A, B) = 0 \text{ for any integer } m \neq k \neq 0. \\ AB \neq \mathbf{0} &\implies \text{tr } S_{m,k}(A, B) > 0 \text{ for any integer } m \geq m_0. \end{aligned}$$

Let us summarize the main idea of the proof. Since the case $AB = \mathbf{0}$ is trivial, we may assume $AB \neq \mathbf{0}$. Moreover, we may assume that A has unit norm.⁴ If now m increases, the k letters B are getting more and more sparsely distributed inside the words in $S_{m,k}(A, B)$. Indeed, most of the terms are of the form $A^{i_1} B A^{i_2} \dots B A^{i_{k+1}}$ with rather large i_ι . These words are approximated by $(P_A B P_A)^k$, where P_A is the hermitian projector $\lim_{i \rightarrow \infty} A^i$. The assertion follows unless $\text{tr } (P_A B)^k$ vanishes. But, then $A = \mathbf{1}_{n-l} \oplus A'$ and $B = \mathbf{0}_{n-l} \oplus B'$ for some positive hermitian $l \times l$ matrices A', B' with $0 < l < n$, such that the proof follows inductively.

Unfortunately, the dependence of m_0 on A and B is crucial for our proof of the theorem. Therefore, the full BMV conjecture does not follow directly from the theorem above. Nevertheless, some (admittedly, simple) numerical simulations indicate further structures in the sequence of $\text{tr } S_{m,k}(A, B)$ for general k . To see them, we should first factor out the trivial dependencies. In fact, observe that otherwise this term (in general) diverges; we have, e.g., $\text{tr } S_{m,k}(\kappa \mathbf{1}, \lambda \mathbf{1}) = n \kappa^{m-k} \lambda^k \binom{m}{k}$. Thus, we will study the normalized quotient

$$q_{m,k}(A, B) := \frac{\text{tr } S_{m,k}(A, B)}{\text{tr } S_{m,k}(\|A\| \mathbf{1}, \|B\| \mathbf{1})},$$

as the BMV conjecture is now equivalent to $q_{m,k}(A, B) \geq 0$ for all positive hermitian matrices A and B having norm 1. Since the theorem above tells us that $q_{m,k}(A, B) > 0$ for sufficiently large m , the BMV conjecture would now follow if one could establish

Conjecture 1.2 Let A and B be positive hermitian $n \times n$ matrices with $AB \neq \mathbf{0}$. Then, for any fixed $k \in \mathbb{N}$, the sequence

$$(q_{m+k,k}(A, B))_{m \in \mathbb{N}}$$

is decreasing.

³If the dimensions of the matrices $\mathbf{0}$ and $\mathbf{1}$ should be clear from the context, we may refrain from specifying them by writing $\mathbf{0}_n$ and $\mathbf{1}_n$, respectively.

⁴In the main text, we always consider the operator norm. Other norms will be discussed in the context of Euler-Lagrange equations in the appendix.

Despite to the mentioned numerical hints, we have not been able to prove this conjecture analytically. Nevertheless, we have been able to deduce further properties of $q_{m,k}(A, B)$ for large m and general k :

Theorem 1.3 Let $\varepsilon > 0$, let A and B be nonzero positive hermitian matrices, and let d be the dimension of the intersection of the eigenspaces of A and B w.r.t. their highest eigenvalues. Then there are $m_0, k_0 > 0$, such that

$$q_{m,k}(A, B) > \frac{d}{n} - \varepsilon \quad \text{for } m \geq m_0 \text{ and } k, m - k \geq 0$$

and

$$q_{m,k}(A, B) < \frac{d}{n} + \varepsilon \quad \text{for } m \geq m_0 \text{ and } k, m - k \geq k_0.$$

In particular, $\text{tr } S_{m,k}(A, B)$ is strictly positive for all k , provided m is sufficiently large and the matrices A and B share a common eigenvector w.r.t. the respective maximal nonzero eigenvalue.

Let us now sketch the idea of the proof for normalized A and B . If $d > 0$, we may decompose A and B into $A' \oplus \mathbf{1}_d$ and $B' \oplus \mathbf{1}_d$, respectively, where A' and B' are positive hermitian with $\|A'B'\| < 1$. Since

$$\begin{aligned} \text{tr } S_{m,k}(A, B) &= \text{tr } S_{m,k}(A', B') + \text{tr } S_{m,k}(\mathbf{1}_d, \mathbf{1}_d) \\ &= \text{tr } S_{m,k}(A', B') + \frac{d}{n} \text{tr } S_{m,k}(\mathbf{1}_n, \mathbf{1}_n), \end{aligned}$$

we may assume $d = 0$, i.e., $\|AB\| < 1$. Moreover, by Theorem 1.1, we may assume that k and $m - k$ are not too small. Now, the typical element among the $S_{m,k}(A, B)$ terms contains a higher and higher number of subwords AB . The norm estimate $\|AB\| < 1$ implies that $q_{m,k}(A, B)$, hence, the average contribution of a word to $S_{m,k}(A, B)$ is getting arbitrarily small.

Our paper is organized as follows: First, for completion, we collect some simple properties of normalized positive hermitian matrices. Then we use combinatorial methods to calculate the number of words in A and B containing the subword AB a certain number of times, and derive estimates for these figures. In Section 4, we prove the estimates announced in the theorems above. Finally, in Appendix A, we derive the Euler-Lagrange equations in a slightly more abstract way than in [6] and extend these results to several norms.

2 Some Algebra

In this section we review the asymptotic behaviour of powers of positive hermitian matrices as well as of their products. Most importantly, we will recall that A^i for unit-norm matrices A always tends to the projector⁵ onto the highest eigenspace (i.e., for the eigenvalue 1); powers of matrix products converge to projectors to common highest eigenspaces. Moreover, we derive some norm and trace estimates as well as some criteria for the product of two matrices to vanish.

2.1 Power Limits

Definition 2.1 For any $n \times n$ matrix A , define $P_A := \lim_{i \rightarrow \infty} A^i$, if the limit exists.

Obviously, we have $P_{\mathbf{1}} = \mathbf{1}$ and $P_{\mathbf{0}} = \mathbf{0}$.

⁵Throughout the whole paper, any projector is assumed to be a hermitian projector.

Lemma 2.1 Let A be any $n \times n$ matrix, such that P_A exists. Then we have:

- P_A is idempotent;
- $AP_A = P_A = P_AA$;
- $P_Ax = x \iff Ax = x$, where $x \in \mathbb{C}^n$;
- $P_{U^{-1}AU}$ exists for any invertible $n \times n$ matrix U , and it equals $U^{-1}P_AU$.

The final statement implies that we often may restrict ourselves to the case of diagonal A , as long as we investigate P_A for hermitian A .

Proof We have

$$\begin{aligned} P_AP_A &= (\lim_{i \rightarrow \infty} A^i)(\lim_{j \rightarrow \infty} A^j) = \lim_{i \rightarrow \infty} (A^i(\lim_{j \rightarrow \infty} A^j)) \\ &= \lim_{i \rightarrow \infty} (\lim_{j \rightarrow \infty} A^{i+j}) = \lim_{i \rightarrow \infty} P_A = P_A \end{aligned}$$

and, similarly, $AP_A = P_A = P_AA$. Now, $x = P_Ax$ implies

$$Ax = A(P_Ax) = (AP_A)x = P_Ax = x.$$

The remaining assertions are obvious.

qed

Definition 2.2 Let A be any $n \times n$ matrix.

Then $I_\lambda(A)$ denotes its eigenspace in \mathbb{C}^n for the eigenvalue λ .

Lemma 2.2 If A is hermitian with $\|A\| \leq 1$ and if -1 is not in the spectrum of A , then P_A exists and is a projector. Moreover, $\text{im } P_A = I_1(A)$.

Proof Consider A in diagonal form and use Lemma 2.1.

qed

Lemma 2.3 Let A_1 be an $n_1 \times n_1$ matrix and A_2 be an $n_2 \times n_2$ matrix, such that P_{A_1} and P_{A_2} exist. Then $P_{A_1 \oplus A_2}$ exists and equals $P_{A_1} \oplus P_{A_2}$.

Proof Use that $(A_1 \oplus A_2)^i = A_1^i \oplus A_2^i$.

qed

2.2 Phone Matrices

Definition 2.3 A matrix A is called **n -phone** iff A is a positive, hermitian $n \times n$ matrix whose largest eigenvalue is 1.

Recall that the norm of a positive hermitian matrix coincides with its largest eigenvalue.

Lemma 2.4 Any nonzero projector is an n -phone matrix.

Lemma 2.5 For any $k \in \mathbb{N}$ and any n -phone matrix A , we have $\|A^k - P_A\| = \|A - P_A\|^k$.

Proof Diagonalize A .

qed

Occasionally, we will decompose matrices into direct sums of matrices. When we simply state that some matrix B equals $B_1 \oplus B_2$, then we tacitly assume that there is some decomposition of \mathbb{C}^n into $X_1 \oplus X_2 \cong \mathbb{C}^{\dim X_1} \oplus \mathbb{C}^{\dim X_2}$, such that $B|_{X_i} = B_i : X_i \longrightarrow X_i$. Furthermore, note that whenever we decompose several matrices into direct sums, we will always assume that all these matrices are decomposed w.r.t. one and the same decomposition of \mathbb{C}^n .

Lemma 2.6 Let A be an n -phone matrix and let $P_A = \mathbf{1}_{n-l} \oplus \mathbf{0}_l$ for some $0 \leq l \leq n$.

Then there is some $0 \leq \alpha < 1$ and some l -phone matrix A' , such that A equals $\mathbf{1}_{n-l} \oplus \alpha A'$. Moreover, we have $l > 0$, unless $A = \mathbf{1}_n$, and $l < n$.

Proof • If $l = n$, then $P_A = \mathbf{0}_n$, whence $I_1(A) = 0$ by Lemma 2.2, i.e., $\|A\| < 1$.
• If $l = 0$, we have $P_A = \mathbf{1}_n$, i.e., $I_1(A) = I_1(P_A) = n$ and, therefore, $A = \mathbf{1}_n$.
• If $0 < l < n$, then $P_A = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$. Let $A = \begin{pmatrix} F & G^* \\ G & H \end{pmatrix}$ with positive hermitian matrices F (of size $n-l$) and H (of size l). From $P_A A = P_A$, we derive $F = \mathbf{1}$ and $G = \mathbf{0}$, whence $A = \mathbf{1}_{n-l} \oplus H$. By

$$\mathbf{1}_{n-l} \oplus \mathbf{0}_l = P_A = P_{\mathbf{1}_{n-l} \oplus H} = P_{\mathbf{1}_{n-l}} \oplus P_H = \mathbf{1}_{n-l} \oplus P_H,$$

we have $P_H = \mathbf{0}_l$, whence $\|H\| < 1$, again by Lemma 2.2. Now, define $\alpha := \|H\|$ and $A' := \alpha^{-1}H$ (or $A' = \mathbf{1}_l$ if $H = \mathbf{0}_l$). **qed**

Corollary 2.7 For any n -phone matrix A , we have $\|A - P_A\| < 1$.

2.2.1 Shared Eigenspaces

Lemma 2.8 Let A_1, \dots, A_N be n -phone matrices and let $x \in \mathbb{C}^n$. Then

$$\|A_N \cdots A_1 x\| = \|x\| \iff A_i x = x \text{ for all } i = 1, \dots, N.$$

Proof We may assume that $x \neq 0$. Moreover, the \Leftarrow direction is trivial. We now prove the \Rightarrow statement by induction. Let $N = 1$ and denote shortly $A := A_1$. Then there is a unitary U , such that $D := UAU^*$ is diagonal. Setting $y := Ux$, we have

$$\|Dy\| \equiv \|UAU^*Ux\| = \|Ax\| = \|x\| = \|Ux\| \equiv \|y\|.$$

Writing $D =: \text{diag}(d_1, \dots, d_n)$ with $0 \leq d_j \leq 1$ and $y =: (y_1, \dots, y_n)^T$, we find that $Dy = (d_1 y_1, \dots, d_n y_n)^T$, whence

$$\sum_{j=1}^n (1 - d_j^2) |y_j|^2 = \sum_{j=1}^n |y_j|^2 - \sum_{j=1}^n d_j^2 |y_j|^2 = \|y\|^2 - \|Dy\|^2 = 0.$$

Since $0 \leq d_j \leq 1$, we have $(1 - d_j^2) |y_j|^2 = 0$ for all j . Consequently,

$$\begin{aligned} d_j = 1 \text{ or } y_j = 0 \text{ for all } j &\implies (d_j - 1)y_j = 0 \text{ for all } j \\ &\implies d_j y_j = y_j \text{ for all } j \\ &\implies Dy = y. \end{aligned}$$

Now, $Ax = U^* D U U^* y = U^* Dy = U^* y = x$.

Next, let $N > 1$ and assume the assertion to be proven for $N - 1$. We now have

$$\begin{aligned} \|x\| &= \|A_N A_{N-1} \cdots A_1 x\| \leq \|A_N\| \|A_{N-1} \cdots A_1 x\| \\ &= \|A_{N-1} \cdots A_1 x\| \leq \|A_{N-1}\| \cdots \|A_1\| \|x\| = \|x\|, \end{aligned}$$

whence $\|A_{N-1} \cdots A_1 x\| = \|x\|$. By induction, $A_i x = x$ for all $i < N$. On the other hand, this implies $\|A_N x\| = \|A_N A_{N-1} \cdots A_1 x\| = \|x\|$. From the induction beginning, we get $A_N x = x$ as well. **qed**

Corollary 2.9 For any n -phone matrices A_1, \dots, A_N we have

$$I_1(A_1 \cdots A_N) = I_1(A_1) \cap \dots \cap I_1(A_N).$$

Proof • Let $x \in I_1(A_1 \cdots A_N)$, i.e. $A_1 \cdots A_N x = x$. Lemma 2.8 implies $A_i x = x$ for all i .
• Trivial. **qed**

Corollary 2.10 For any n -phone matrices A_1, \dots, A_N we have

$$I_1(A_1 \cdots A_N) \neq \emptyset \iff \|A_1 \cdots A_N\| = 1.$$

Proof • If $\|A_1 \cdots A_N\| = 1$, then there is some nonzero $x \in \mathbb{C}^n$ with $\|A_1 \cdots A_N x\| = \|x\|$. Lemma 2.8 implies that $A_i x = x$ for all i . This, of course, implies $A_1 \cdots A_N x = x$.
 • If $I_1(A_1 \cdots A_N) \neq 0$, then, by Corollary 2.9, there is some nonzero $x \in \mathbb{C}^n$, such that $A_i x = x$ for all i . Now, $A_1 \cdots A_N x = x$ and $\|A_1 \cdots A_N\| = 1$. **qed**

Corollary 2.11 Let A_1, \dots, A_N be n -phone matrices. Then we have:

$$P_{A_1 \cdots A_N} \text{ exists and equals } \mathbf{0}. \iff I_1(A_1 \cdots A_N) = 0.$$

Proof • If $I_1(A_1 \cdots A_N) = 0$, then, by Corollary 2.10, $\|A_1 \cdots A_N\| < 1$, whence we have $\|(A_1 \cdots A_N)^j\| \leq \|A_1 \cdots A_N\|^j \rightarrow 0$ for $j \rightarrow \infty$. Consequently, $P_{A_1 \cdots A_N} = \mathbf{0}$.
 • If $I_1(A_1 \cdots A_N) \neq 0$, then, by Corollary 2.9, there is some nonzero $x \in \mathbb{C}^n$, such that $A_i x = x$ for all i . This means, $A_1 \cdots A_N x = x$ and thus $P_{A_1 \cdots A_N} x = x$. **qed**

Lemma 2.12 For any n -phone matrices A_1, \dots, A_N we have:

1. There are $n' \times n'$ matrices A'_1, \dots, A'_N , such that for $i = 1, \dots, N$
 - $A_i = A'_i \oplus \mathbf{1}_l$,
 - each A'_i is positive hermitian;
 - $\|A'_1 \cdots A'_N\| < 1$.
 Here, $l := \dim I_1(A_1 \cdots A_N)$ and $n' := n - l$.
2. $P_{A_1 \cdots A_N}$ exists and is the projector to $I_1(A_1 \cdots A_N)$.

Proof Denote $I_1(A_1 \cdots A_N) \subseteq \mathbb{C}^n$ shortly by X . By Corollary 2.9, each A_i is the identity when restricted to X . Since each A_i is hermitian, X^\perp is preserved by each A_i .⁶ Hence, we may decompose each A_i into $\mathbf{1}_X \oplus A'_i$ according to $\mathbb{C}^n = X \oplus X^\perp$. Here, A'_i is a positive, hermitian operator on X^\perp . (W.l.o.g., we may assume that A'_i is an $n' \times n'$ matrix with $n' := n - \dim X$.) If $\|A'_1 \cdots A'_N\|$ was 1, then

$$1 = \|A'_1 \cdots A'_N\| \leq \|A'_1\| \cdots \|A'_N\| \leq 1,$$

and each A'_i would be n -phone. Since, however, by construction and by Corollary 2.9, $0 = I_1(A'_1) \cap \dots \cap I_1(A'_N) = I_1(A'_1 \cdots A'_N)$, we have $P_{A'_1 \cdots A'_N} = \mathbf{0}$, as shown in Corollary 2.11. Consequently, by Corollary 2.10, $\|A'_1 \cdots A'_N\| \neq 1$. Obviously, we have $P_{\mathbf{1}_X} = \mathbf{1}_X$, such that, by Lemma 2.3, $P_{A_1 \cdots A_N} = P_{(\mathbf{1}_X \oplus A'_1) \cdots (\mathbf{1}_X \oplus A'_N)}$ exists and equals $P_{\mathbf{1}_X} \oplus P_{A'_1 \cdots A'_N} = \mathbf{1}_X \oplus \mathbf{0}_{X^\perp}$. It is, of course, hermitian. **qed**

Corollary 2.13 $I_1(A_1 \cdots A_N) = I_1(P_{A_1 \cdots A_N})$ for any n -phone matrices $A_1 \cdots A_N$.

2.2.2 Norms and Traces

Lemma 2.14 Let A, B be n -phone matrices. Then $\|AB^i A\| \leq \|AB^j A\|$ for all $i \geq j$.

Proof Let D be the n -phone matrix with $B = D^2$. Then

$$\|AB^i A\| = \|(D^i A)^*(D^i A)\| = \|D^i A\|^2 \leq \|D^{i-j}\|^2 \|D^j A\|^2 = \|AB^j A\|.$$

qed

Corollary 2.15 Let A, B be n -phone matrices.

Then $ABA = \mathbf{0}$ implies $AB^i A = \mathbf{0}$ for any $i \in \mathbb{N}_+$.

Proof We have $0 = \|ABA\| \geq \|AB^i A\| \geq 0$ by Lemma 2.14. **qed**

⁶Let $x^\perp \in X^\perp$ and $x \in X$. Then $\langle x, A_i x^\perp \rangle = \langle A_i^* x, x^\perp \rangle = \langle A_i x, x^\perp \rangle = \langle x, x^\perp \rangle = 0$, hence $A_i x^\perp \in X^\perp$.

Lemma 2.16 For any n -phone matrices A and B , we have

$$\|BAB\|^{k+1} \leq \|(AB^2)^k\| \leq \|BAB\|^{k-1}.$$

If B is even a projector P , then

$$\|PAP\|^k \leq \|(AP)^k\| \leq \|PAP\|^{k-1}.$$

Proof Since $BAB = B^*AB$ is hermitian and positive, we have $\|(BAB)^k\| = \|BAB\|^k$ for any $k \in \mathbb{N}$. Now observe that

$$\begin{aligned} \|BAB\|^{k+1} &= \|(BAB)^{k+1}\| = \|B(AB^2)^k AB\| \\ &\leq \|(AB^2)^k\| = \|AB(BAB)^{k-1}B\| \\ &\leq \|(BAB)^{k-1}\| = \|BAB\|^{k-1}, \end{aligned}$$

since $\|A\| = 1 = \|B\|$ and, similarly,

$$\begin{aligned} \|PAP\|^k &= \|(PAP)^k\| = \|P(AP)^k\| \leq \|(AP)^k\| = \|AP(AP)^{k-1}\| \\ &\leq \|P(AP)^{k-1}\| = \|(PAP)^{k-1}\| = \|PAP\|^{k-1}, \end{aligned}$$

since $P^2 = P$ and $\|P\| = 1$.

qed

Proposition 2.17 Let A and B be n -phone matrices, and let $k \in \mathbb{N}_+$. Then

$$AB = \mathbf{0} \iff \operatorname{tr} AB = 0 \iff \operatorname{tr} (AB)^k = 0 \iff ABA = \mathbf{0}.$$

Proof Let C be an n -phone matrix with $A = C^2$.

- First of all, let $\operatorname{tr} (AB)^k = 0$ for some $k \in \mathbb{N}_+$. Since

$$\operatorname{tr} (AB)^k = \operatorname{tr} C(CBC)^{k-1}CB = \operatorname{tr} (CBC)^k$$

and since CBC is positive hermitian, we have⁷ $CBC = \mathbf{0}$ and $ABA = \mathbf{0}$.

- Next, $ABA = \mathbf{0}$ implies $(BA)^*BA \equiv AB^2A = \mathbf{0}$ by Corollary 2.15, whence $\|BA\|^2 = \|(BA)^*BA\| = 0$, implying $BA = \mathbf{0}$ and $AB = \mathbf{0}$.
- Finally, of course, $AB = \mathbf{0}$ implies $\operatorname{tr} (AB)^k = 0$.

qed

2.2.3 Splitting

Lemma 2.18 Let A and B be n -phone matrices. Then $AB = \mathbf{0}$ iff there is some $0 < l < n$, some l -phone matrix A' and some $(n-l)$ -phone matrix B' , such that

$$A = A' \oplus \mathbf{0}_l \quad \text{and} \quad B = \mathbf{0}_{n-l} \oplus B'.$$

Note again, the splitting above means that there is a basis of \mathbb{C}^n , such that A and B can be simultaneously splitted in the way given above.

Proof If A and B can be split in the given way, then AB obviously vanishes. The other way round, $AB = \mathbf{0}$ implies $BA = \mathbf{0}$, hence $AB = BA$, whence A and B can be diagonalized simultaneously. Now, the statement is trivial. **qed**

Lemma 2.19 Let $k \in \mathbb{N}_+$, and let A and B be n -phone matrices.

Then we have $\operatorname{tr} (P_A B)^k = 0$ iff there are $0 \leq \alpha < 1$, $0 < l < n$ and l -phone matrices A' and B' with

$$A = \mathbf{1}_{n-l} \oplus \alpha A' \quad \text{and} \quad B = \mathbf{0}_{n-l} \oplus B'.$$

⁷ $\operatorname{tr} D^k = 0$ implies $D = \mathbf{0}$ for positive hermitian matrices D .

Proof By Proposition 2.17, $\text{tr}(P_A B)^k = 0$ is equivalent to $P_A B = \mathbf{0}$. Analogously to the proof of Lemma 2.18, we see that, for $P_A B = \mathbf{0}$, there is a decomposition

$$P_A = \mathbf{1}_{n-l} \oplus \mathbf{0}_l \quad \text{and} \quad B = \mathbf{0}_{n-l} \oplus B'$$

for some l -phone matrix B' . Since $P_A \neq \mathbf{1}$ by $P_A B = \mathbf{0}$, we have $0 < l < n$. Now the implication follows from Lemma 2.6. The other direction is trivial. **qed**

3 Some Combinatorics

The ultimate goal of this article is to derive asymptotic properties of $\text{tr} S_{m,k}(A, B)$. Recall that $S_{m,k}(A, B)$ equals the sum of all products of matrices where $m - k$ factors equal A and k factors equal B . The trace of such a single product significantly depends on its “factor pattern”. For instance, if the substring AB appears l times in the matrix product, then the trace of the full product cannot exceed $n\|AB\|^l$. To finally estimate the sum of all these product traces, we need estimates how frequently this pattern appears. This now is a purely combinatorial problem for words in two letters. To avoid confusion we will denote the letters by a and b , and return to A and B only later. Let, moreover, $0 \leq k \leq m$ be integers and denote the set of all words containing exactly $m - k$ letters a and k letters b by $\mathcal{W}_{m,k}$.

3.1 Counting

Proposition 3.1 Denote by $\mathcal{C}_{m,k,s} \subseteq \mathcal{W}_{m,k}$ the set of words containing exactly s times the subword ab . Then we have

$$|\mathcal{C}_{m,k,s}| = \binom{m-k}{s} \binom{k}{s}$$

and

$$|\mathcal{W}_{m,k}| = \sum_s |\mathcal{C}_{m,k,s}| = \binom{m}{k}.$$

Here, we used the convention that $\binom{i}{j} = 0$ if $j > i$.

Proof Let $w \in \mathcal{C}_{m,k,s}$ be a word with exactly s subwords ab . Then

$$w = b^{j_0} a^{i_1} b^{j_1} \dots a^{i_s} b^{j_s} a^{i_{s+1}}$$

for appropriate $i_\iota, j_\iota \geq 1$, $\iota = 1, \dots, s$, and $j_0, i_{s+1} \geq 0$ with $i_1 + \dots + i_{s+1} = m - k$ and $j_0 + \dots + j_s = k$. Obviously, it is sufficient to prove that there are exactly $\binom{k}{s}$ ways to write k as a sum $j_0 + j_1 + \dots + j_s$ of $s + 1$ integers with $j_0 \geq 0$ and $j_\iota \geq 1$. In fact, there are $\binom{k}{s}$ possibilities to choose s elements $J_1 < \dots < J_s$ out of the k numbers $1, \dots, k$. Letting $j_0 := J_1 - 1$ and $j_\iota := J_{\iota+1} - J_\iota$ for $0 < \iota < s$ and $j_s := k + 1 - J_s$ gives such a decomposition $j_0 + j_1 + \dots + j_s$ of k . Since, the other way round, each such decomposition can be obtained by such J_ι , we get the proof. The second assertion is clear. **qed**

Lemma 3.2 1. No word in $\mathcal{C}_{m,k,k}$ contains the subword bb , i.e., any word in $\mathcal{C}_{m,k,k}$ can be written as $a^{i_1} b a^{i_2} \dots a^{i_k} b a^{i_{k+1}}$ with $i_\iota > 0$ and $i_{k+1} \geq 0$.
2. Denote by $\mathcal{D}_{m,k,L} \subseteq \mathcal{C}_{m,k,k}$ the set of those words $a^{i_1} b a^{i_2} \dots a^{i_k} b a^{i_{k+1}}$ as above with $i_\iota > L$ and $i_{k+1} \geq L$ for some integer $L \geq 0$. Then

$$|\mathcal{D}_{m,k,L}| = |\mathcal{C}_{m-(k+1)L,k,k}|.$$

Proof 1. This follows directly from the proof of Proposition 3.1. In fact, let

$$w = b^{j_0} a^{i_1} b^{j_1} \dots a^{i_k} b^{j_k} a^{i_{k+1}} \in \mathcal{C}_{m,k,k}.$$

Since $j_0 + \dots + j_k = k$ and $j_1, \dots, j_k > 0$, we have $j_0 = 0$ and $j_1 = \dots = j_k = 1$.

2. One easily checks that

$$\begin{aligned} \xi : \mathcal{C}_{m-(k+1)L,k,k} &\longrightarrow \mathcal{D}_{m,k,L} \subseteq \mathcal{C}_{m,k,k} \\ a^{i_1} b a^{i_2} \dots a^{i_k} b a^{i_{k+1}} &\longmapsto a^{i_1+L} b a^{i_2+L} \dots a^{i_k+L} b a^{i_{k+1}+L} \end{aligned}$$

is a bijection.

qed

3.2 Estimates

We will need estimates on how the number of words changes in the event of having a fixed amount of letters less and how often there are subwords ab . In the first simple lemma, we will see that the (relative) decrease of the word number for dropping a finite number of letters a is arbitrarily small provided we had started with a occurring sufficiently often. In the second lemma, we show that —again for a occurring sufficiently often, i.e., for large m — the (relative) number of words containing less than k subwords ab can be made arbitrarily small. Or, in other words, if one of the k letters b appears then it appears “lonely”, i.e., b^2 or higher powers typically do not appear.

Lemma 3.3 For $0 < \varepsilon < 1$, positive integers L and m with $m \geq L(1 + \frac{k}{\varepsilon})$, we have

$$\binom{m-L}{k} \geq (1-\varepsilon) \binom{m}{k}.$$

Proof Use

$$\binom{m-L}{k} = \binom{m}{k} \prod_{j=0}^{L-1} \left(1 - \frac{k}{m-j}\right) \geq \binom{m}{k} \prod_{j=0}^{L-1} \left(1 - \frac{\varepsilon}{L}\right) \geq \binom{m}{k} (1-\varepsilon).$$

qed

Lemma 3.4 Let $0 < \varepsilon < 1 \leq S$ and

$$m > \frac{S^3}{\varepsilon} + 2S - 1 \quad \text{and} \quad k, m-k \geq S.$$

Then

$$\sum_{s=0}^{S-1} \binom{m-k}{s} \binom{k}{s} < \varepsilon \binom{m-k}{S} \binom{k}{S}.$$

Proof Observe that for $0 \leq s \leq S \leq k, m-k$ and for m as in the lemma

$$\begin{aligned} \frac{s^2}{\varepsilon} &\leq \frac{S^3}{\varepsilon} \leq \frac{S^3}{\varepsilon} + 2S - 1 - (2s - 1) < m - 2s + 1 \\ &\leq ((m-k) - s)(k-s) + m - 2s + 1 = ((m-k) - s + 1)(k-s + 1). \end{aligned}$$

Using the abbreviation $d_s := \binom{m-k}{s} \binom{k}{s}$ for all $s \in \mathbb{N}$, one immediately checks that

$$d_{s-1} = \frac{s^2}{((m-k-s+1)(k-s+1))} d_s.$$

As just seen above, the prefactor is always smaller than $\varepsilon < 1$, whence we get

$$\sum_{s=0}^{S-1} d_s \leq \sum_{s=0}^{S-1} d_{s-1} = S d_{S-1} = \frac{S^3}{((m-k-S+1)(k-S+1))} d_S < \varepsilon d_S.$$

qed

4 Proofs of the Main Theorems

4.1 Growing m and Fixed k

There are two main steps in the study of the asymptotics of $\text{tr } S_{m,k}(A, B)$ for growing m while k is fixed: First, we estimate how fast the products $A^{l_1}B \cdots A^{l_k}B$ do approach $(P_AB)^k$ depending on the minimal L of all l_i . Second, the longer the words are (i.e., for growing m) all other words (i.e., those with $l_i < L$ or having substrings b^2) get less frequent for fixed L . This allows us to estimate how fast $\text{tr } S_{m,k}(A, B)/\text{tr } S_{m,k}(\mathbf{1}, \mathbf{1})$ approaches $\text{tr } (P_AB)^k/n$ and, finally, to prove Theorem 1.1.

Lemma 4.1 For any n -phone matrices A and B and for any integers $l_1, \dots, l_k \geq L > 0$, we have

$$\left\| \prod_{i=1}^k A^{l_i} B - \prod_{i=1}^k P_A B \right\| \leq k \|A - P_A\|^L \|A^L B\|^{k-1}.$$

Proof Observe that for any $n \times n$ matrices X_1, \dots, X_k and X , we have (see Lemma C.1)

$$X_1 \cdots X_k = X^k + \sum_{i=1}^k X^{i-1} (X_i - X) X_{i+1} \cdots X_k.$$

Now, Lemma 2.5 implies

$$\begin{aligned} \left\| \prod_{i=1}^k A^{l_i} B - \prod_{i=1}^k P_A B \right\| &\leq \sum_{i=1}^k \|(P_AB)^{i-1}\| \|(A^{l_i} - P_A)B\| \|A^{l_{i+1}}B\| \cdots \|A^{l_k}B\| \\ &\leq \sum_{i=1}^k \|P_AB\|^{i-1} \|A - P_A\|^{l_i} \|A^{l_{i+1}}B\| \cdots \|A^{l_k}B\| \\ &\leq \|A - P_A\|^L \sum_{i=1}^k \|A^L B\|^{i-1} \|A^L B\|^{k-i} \\ &= k \|A - P_A\|^L \|A^L B\|^{k-1}. \end{aligned}$$

qed

In Section 3, we studied words in the two letters a and b . We now define W to be the homomorphism from $\mathcal{W}_{m,k}$ to the $n \times n$ matrices, whereas $W(a) := A$ and $W(b) := B$. It is now clear that, e.g., $S_{m,k}(A, B) = \sum_{w \in \mathcal{W}_{m,k}} W(w)$.

Proposition 4.2 Let A and B be n -phone matrices, and let $k \in \mathbb{N}$ and $\varepsilon \in (0, 1)$ be fixed. Choose now some $L \in \mathbb{N}_+$, such that

$$k \|A - P_A\|^L \|A^L B\|^{k-1} < \varepsilon.$$

Then, for any $m \in \mathbb{N}$ with

$$m \geq \left(1 + \frac{k}{\varepsilon}\right) (k + kL + L),$$

we have

$$\left| \frac{\text{tr } S_{m,k}(A, B)}{\text{tr } S_{m,k}(\mathbf{1}, \mathbf{1})} - \frac{\text{tr } (P_AB)^k}{n} \right| \leq \left(\frac{\text{tr } (P_AB)^k}{n} + 2 \right) \varepsilon.$$

Observe that $\text{tr } (P_AB)^k$ is always nonnegative.

Proof First observe, that $\|A - P_A\| < 1$ by Corollary 2.7, whence there exists such an L . Next, observe that

$$\begin{aligned}
|\mathcal{W}_{m,k} \setminus \mathcal{D}_{m,k,L}| &= |\mathcal{W}_{m,k}| - |\mathcal{D}_{m,k,L}| \\
&= |\mathcal{W}_{m,k}| - |\mathcal{C}_{m-(k+1)L,k,k}| && \text{(by Lemma 3.2)} \\
&= \binom{m}{k} - \binom{m-(k+1)L-k}{k} \binom{k}{k} && \text{(by Proposition 3.1)} \\
&\leq \binom{m}{k} - (1-\varepsilon) \binom{m}{k} && \text{(by Lemma 3.3)} \\
&= \varepsilon |\mathcal{W}_{m,k}|.
\end{aligned}$$

since $m \geq ((k+1)L+k)(1+\frac{k}{\varepsilon})$ by assumption. Third, observe that for $w \in \mathcal{D}_{m,k,L}$, we have

$$|\operatorname{tr} W(w) - \operatorname{tr} (P_A B)^k| \leq nk \|A - P_A\|^L \|A^L B\|^{k-1} < n\varepsilon$$

by Lemma 4.1 and $|\operatorname{tr} C| \leq n\|C\|$ for any matrix C , whence

$$\begin{aligned}
&\left| \frac{\sum_{w \in \mathcal{W}_{m,k}} \operatorname{tr} W(w)}{\operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} - \frac{\operatorname{tr} (P_A B)^k}{n} \right| \\
&= \left| \sum_{w \in \mathcal{W}_{m,k}} \frac{\operatorname{tr} W(w) - \operatorname{tr} (P_A B)^k}{\operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} \right| \\
&\leq \left| \sum_{w \in \mathcal{D}_{m,k,L}} \frac{\operatorname{tr} W(w) - \operatorname{tr} (P_A B)^k}{\operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} \right| + \sum_{w \in \mathcal{W}_{m,k} \setminus \mathcal{D}_{m,k,L}} \left| \frac{\operatorname{tr} W(w) - \operatorname{tr} (P_A B)^k}{\operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} \right| \\
&< \frac{|\mathcal{D}_{m,k,L}|}{n|\mathcal{W}_{m,k}|} n\varepsilon + \frac{|\mathcal{W}_{m,k}| - |\mathcal{D}_{m,k,L}|}{n|\mathcal{W}_{m,k}|} (n + |\operatorname{tr} (P_A B)^k|) \\
&< \left(2 + \frac{\operatorname{tr} (P_A B)^k}{n} \right) \varepsilon
\end{aligned}$$

using

$$|\mathcal{W}_{m,k}| = \binom{m}{k} = \sum_{w \in \mathcal{W}_{m,k}} 1 = \frac{1}{n} \operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1}).$$

qed

Theorem 1.1 is now a corollary:

Proof Theorem 1.1

We may assume that A and B are n -phone matrices and that $k \neq 0$. We proceed partially by induction. The case of $n = 1$ is trivial as well as the case $AB = \mathbf{0}$. Let now $n > 1$ and $AB \neq \mathbf{0}$.

- Assume first that $\operatorname{tr} (P_A B)^k > 0$. Then there are $L > 0$ and $\varepsilon \in (0, 1)$ with

$$k \|A - P_A\|^L \|A^L B\|^{k-1} < \varepsilon < \frac{\operatorname{tr} (P_A B)^k}{3n}.$$

Now, since $0 < \operatorname{tr} (P_A B)^k \leq n$, we have

$$\begin{aligned}
\frac{\operatorname{tr} S_{m,k}(A, B)}{\operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} &\geq \frac{\operatorname{tr} (P_A B)^k}{n} - \left(\frac{\operatorname{tr} (P_A B)^k}{n} + 2 \right) \varepsilon \\
&> \frac{\operatorname{tr} (P_A B)^k}{n} - \left(\frac{\operatorname{tr} (P_A B)^k}{n} + 2 \right) \frac{\operatorname{tr} (P_A B)^k}{3n} \\
&= \frac{1}{3} \frac{\operatorname{tr} (P_A B)^k}{n} \left(1 - \frac{\operatorname{tr} (P_A B)^k}{n} \right) \geq 0,
\end{aligned}$$

provided

$$m \geq m_0 := \left(1 + \frac{k}{\varepsilon}\right) (k + kL + L).$$

The assertion follows, since $\text{tr}(P_A B)^k > 0$ implies $P_A B P_A \neq \mathbf{0}$, whence $AB \neq \mathbf{0}$.

- Assume now that $\text{tr}(P_A B)^k = 0$. Then, by Lemma 2.19, we find some $0 \leq \alpha < 1$ and some l -phone matrices A' and B' with $0 < l < n$, such that

$$A = \mathbf{1}_{n-l} \oplus \alpha A' \quad \text{and} \quad B = \mathbf{0}_{n-l} \oplus B'.$$

Since $\mathbf{0} \neq AB = \mathbf{0}_{n-l} \oplus \alpha A' B'$, we have $\alpha \neq 0$ and $A' B' \neq \mathbf{0}_l$. Together with

$$S_{m,k}(A, B) = S_{m,k}(\mathbf{1}_{n-l}, \mathbf{0}_{n-l}) + \alpha^{m-k} S_{m,k}(A', B') = \alpha^{m-k} S_{m,k}(A', B')$$

by Lemma 4.3 and $k > 0$, this implies the assertion by induction. qed

Lemma 4.3 Let A_i and B_i be hermitian $n_i \times n_i$ matrices with $n_i \in \mathbb{N}$ for $i = 1, 2$. Then

$$S_{m,k}(A_1 \oplus \alpha A_2, B_1 \oplus \beta B_2) = S_{m,k}(A_1, B_1) + \alpha^{m-k} \beta^k S_{m,k}(A_2, B_2)$$

for all $m, k \in \mathbb{N}$ and $\alpha, \beta \in \mathbb{C}$.

Proof Obvious. qed

Remark The proof of Theorem 1.1 above provides us with an explicit estimate for the value of m_0 . If A is not a projector and $P_A B \neq \mathbf{0}$, we have $\text{tr} S_{m,k}(A, B) > 0$ for all $m \geq m_0$ with

$$m_0 := (1 + k) \left(1 + \frac{3kn}{\text{tr}(P_A B)^k}\right) \left(2 + \frac{\ln \text{tr}(P_A B)^k - \ln 3kn}{\ln \|A - P_A\|}\right).$$

If A is a projector and $AB \neq \mathbf{0}$, then $\text{tr} S_{m,k}(A, B) > 0$ for all $m \geq m_0$ with

$$m_0 := (1 + 2k) \left(1 + \frac{3kn}{\text{tr}(AB)^k}\right).$$

For $P_A B = \mathbf{0}$, use the decompositions of A and B as in the proof of the theorem and then use the expressions above with A and B replaced by A' and B' , respectively. (If again $P_{A'} B' = \mathbf{0}$, proceed iteratively.) Of course, the estimates above need not be optimal; if the BMV conjecture was true, m_0 would probably be k unless $AB = 0$.

4.2 Growing m and Not-too-small k

If ab appears S times in a word in $\mathcal{W}_{m,k}$, then the corresponding matrix product has at most norm $\|AB\|^S$. For growing m , the typical number of alternations between a and b in a word indeed increases; in particular, it passes the threshold S sooner or later. Therefore, the normalized trace of $S_{m,k}(A, B)$ can be estimated by $\|AB\|^S$ up to some ε .

Proposition 4.4 Let $0 < \varepsilon < 1 \leq S$ for some $S \in \mathbb{N}$ and

$$m > \frac{S^3}{\varepsilon} + 2S - 1 \quad \text{and} \quad k, m - k \geq S.$$

Then

$$\left| \frac{\text{tr} S_{m,k}(A, B)}{\text{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} \right| < \varepsilon + \|AB\|^S.$$

Proof First observe that $|\text{tr } W(w)| \leq n \|W(w)\| \leq n \|AB\|^S$ for any $w \in \mathcal{D}_{m,k,s}$ with $s \geq S$. Now, we simply decompose all elements of $\mathcal{W}_{m,k}$ into two sets: one consisting of all elements containing less than S subwords ab and the other one consisting of all elements with at least S subwords ab . We get

$$\begin{aligned}
|\text{tr } S_{m,k}(A, B)| &\leq \sum_{s < S} \sum_{w \in \mathcal{C}_{m,k,s}} |\text{tr } W(w)| + \sum_{s \geq S} \sum_{w \in \mathcal{C}_{m,k,s}} |\text{tr } W(w)| \\
&\leq \sum_{s < S} |\mathcal{C}_{m,k,s}| n + \sum_{s \geq S} \sum_{w \in \mathcal{C}_{m,k,s}} n \|AB\|^S \\
&< \varepsilon |\mathcal{C}_{m,k,S}| n + |\mathcal{W}_{m,k}| n \|AB\|^S \quad (\text{by Lemma 3.4}) \\
&\leq n |\mathcal{W}_{m,k}| (\varepsilon + \|AB\|^S) \\
&\leq \text{tr } S_{m,k}(\mathbf{1}, \mathbf{1}) (\varepsilon + \|AB\|^S).
\end{aligned}$$

qed

4.3 Asymptotics for Growing m and General k

Since $I_1(A) \cap I_1(B) = I_1(AB)$, Theorem 1.3 follows immediately from

Theorem 4.5 For any n -phone matrices A and B , and for any $0 < \varepsilon < 1$, there are some $m_0 \in \mathbb{N}$ and some $k_0 \in \mathbb{N}$, such that for all $m \geq m_0$

$$\frac{\text{tr } S_{m,k}(A, B)}{\text{tr } S_{m,k}(\mathbf{1}, \mathbf{1})} > \frac{\dim I_1(AB)}{n} - \varepsilon \quad \text{for all } 0 \leq k \leq m$$

and

$$\frac{\text{tr } S_{m,k}(A, B)}{\text{tr } S_{m,k}(\mathbf{1}, \mathbf{1})} < \frac{\dim I_1(AB)}{n} + \varepsilon \quad \text{for all } k_0 \leq k \leq m - k_0.$$

Proof First of all, let us find k_0 and m'_0 , such that

$$\left| \frac{\text{tr } S_{m,k}(A, B)}{\text{tr } S_{m,k}(\mathbf{1}, \mathbf{1})} - \frac{\dim I_1(AB)}{n} \right| < \varepsilon$$

for all $m \geq m'_0$ and $k_0 \leq k \leq m - k_0$.

- Assume first $\|AB\| < 1$, i.e., $I_1(AB) = 0$ by Corollary 2.10. Choose some integer k_0 , such that

$$\|AB\|^{k_0} < \frac{\varepsilon}{2},$$

and some $m'_0 \in \mathbb{N}$, such that

$$m'_0 > \frac{2k_0^3}{\varepsilon} + 2k_0 - 1.$$

Now, Proposition 4.4 implies that

$$\left| \frac{\text{tr } S_{m,k}(A, B)}{\text{tr } S_{m,k}(\mathbf{1}, \mathbf{1})} \right| < \varepsilon$$

for all $m \geq m'_0$ and all $k_0 \leq k \leq m - k_0$.

- Assume now $\|AB\| = 1$. According to Lemma 2.12, we may decompose A and B into $A = A' \oplus \mathbf{1}_l$ and $B = B' \oplus \mathbf{1}_l$ with $\|A'B'\| < 1$ for $l := \dim I_1(AB)$. Using Lemma 4.3, we have

$$\text{tr } S_{m,k}(A, B) = \text{tr } S_{m,k}(A', B') + \text{tr } S_{m,k}(\mathbf{1}_l, \mathbf{1}_l),$$

and, therefore,

$$\frac{\operatorname{tr} S_{m,k}(A, B)}{\operatorname{tr} S_{m,k}(\mathbf{1}_n, \mathbf{1}_n)} - \frac{l}{n} = \frac{l}{n} \frac{\operatorname{tr} S_{m,k}(A', B')}{\operatorname{tr} S_{m,k}(\mathbf{1}_l, \mathbf{1}_l)}.$$

- If $\|A'\| \|B'\| = 1$, then A' and B' are l -phone matrices with $\|A'B'\| < 1$, for that the result has been established above.
- If $\|A'\| \|B'\| < 1$, then choose $k_0 \in \mathbb{N}$, such that $(\|A'\| \|B'\|)^{k_0} < \varepsilon$. Then, by Lemma 4.3, we have

$$\left| \frac{\operatorname{tr} S_{m,k}(A, B)}{\operatorname{tr} S_{m,k}(\mathbf{1}_n, \mathbf{1}_n)} - \frac{l}{n} \right| \leq \frac{l}{n} \|A'\|^{m-k} \|B'\|^k < \varepsilon$$

for any $m, k \in \mathbb{N}$ with $m - k \geq k_0$ and $k \geq k_0$.

Now, let us finish the proof by showing that

$$\frac{\operatorname{tr} S_{m,k}(A, B)}{\operatorname{tr} S_{m,k}(\mathbf{1}, \mathbf{1})} - \frac{\dim I_1(AB)}{n} \geq 0$$

for all $m \geq m_0$ with an appropriate m_0 and for $k \leq k_0$ or $k \geq m - k_0$.

- Assume again first that $\|AB\| < 1$. Now, according to Theorem 1.1, for each $k \in \mathbb{N}$, there is some integer $m'_0(k)$, such that

$$\operatorname{tr} S_{m,k}(A, B) \geq 0 \quad \text{and} \quad \operatorname{tr} S_{m,m-k}(A, B) \equiv \operatorname{tr} S_{m,k}(B, A) \geq 0$$

for all $m \geq m'_0(k)$. Now, simply define

$$m_0 := \max_{k \leq k_0} \{m'_0(k), m'_0\},$$

and we have the desired assertion.

- If $\|AB\| = 1$, we decompose A and B as above into $A = A' \oplus \mathbf{1}_l$ and $B = B' \oplus \mathbf{1}_l$ with $\|A'B'\| < 1$. Again using Lemma 4.3, the assertion follows as in the previous case. **qed**

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Appendix

A Euler-Lagrange Equations

In the main body of the article, we have always used the operator norm for matrices and reduced our investigations typically to normalized matrices. In fact, this has been justified by the homogeneity of $S_{m,k}(\cdot, \cdot)$. Nevertheless, there is a full range of other possible norms that can be taken to normalize the matrices. In [6], e.g., the Frobenius norm has been used to derive the Euler-Lagrange equations of the BMV conjecture. They yielded, among others, relations between A^2 and $AS_{m-1,k}(A, B)$ in any point where $\operatorname{tr} S_{m,k}$ is minimal or maximal. In this appendix we are going to rederive these relations in a slightly more abstract way and extend them to other norms.

For that purpose, we choose the following Schatten p -norms⁸

$$\|A\|_p := \sqrt[p]{\operatorname{tr} A^p} \quad \text{and} \quad \|A\|_\infty := \|A\|$$

for $p \geq 1$ and for positive hermitian A . One immediately sees that $\|A\|_\infty = \lim_{p \rightarrow \infty} \|A\|_p$. Let us now fix some $p \in [1, \infty]$. Moreover, to avoid cumbersome notation, we let n -phone matrices be positive hermitian matrices having p -norm 1 (instead of to be of operator norm 1 as in the main text). Next, observe that for any matrix-valued functions f and g on \mathbb{R} , we have

$$\frac{d}{dx} \operatorname{tr} (f + tg)^m = m \operatorname{tr} \left(\frac{d(f + tg)}{dx} (f + tg)^{m-1} \right)$$

and, by comparison of coefficients,

$$\operatorname{tr} S'_{m,k}(f, g) = m \operatorname{tr} (f' S_{m-1,k}(f, g) + g' S_{m-1,k-1}(f, g)).$$

Here, we abbreviate $f' := \frac{df}{dx}$, etc. We now use two different types of functions for f and g : on the one hand, we keep the eigenvalues by conjugation with unitary matrices, on the other hand, we modify them by multiplication with appropriate commuting matrices. Namely, let first

$$f(x) := e^{-xC} A e^{xC} \quad \text{for } C \in \mathfrak{su}(n),$$

i.e., $C^* = -C$ and $\operatorname{tr} C = 0$. Then $f(0) = A$ and $f'(0) = [A, C]$. Moreover, $f(x)$ is n -phone for any x and any n -phone A . If now (A, B) is an extremal point for $\operatorname{tr} S_{m,k}$ among the positive matrices with unit p -norm, then we have for all $C \in \mathfrak{su}(n)$

$$0 = \operatorname{tr} S'_{m,k}(f, B)|_{x=0} = m \operatorname{tr} ([A, C] S_{m-1,k}(A, B)).$$

Since A and $S_{m-1,k}(A, B)$ are hermitian [6], we get $[S_{m-1,k}(A, B), A] = \mathbf{0}$ from Lemma B.1. Now, secondly, we consider

$$f(x) := \frac{A e^{xC}}{\|A e^{xC}\|_p} \quad \text{for } C \in \mathfrak{gl}(n).$$

Note that f may fail to be differentiable at $x = 0$ for $p = \infty$. In fact, let E_{ij} be the matrix having entry 1 at position (i, j) and zeros elsewhere. Consider $A := E_{11} + E_{22}$ and $C := E_{11}$. Then $\|A e^{xC}\|$ equals e^x for $x \geq 0$ and 1 for $x \leq 0$, which is obviously not differentiable. In general, the problem arises if the maximal eigenvalue of A is of multiplicity 2 or higher. Therefore, for the moment, we assume p to be finite. One easily⁹ checks that

$$f'(0) = \frac{1}{\|A\|_p^{p+1}} (AC \operatorname{tr} A^p - A \operatorname{tr} A^p C).$$

Of course, a priori, it is not clear that $f(x)$ is positive and hermitian, even for small x . But, if U is some unitary matrix, such that $U^* A U$ (and $U^* S_{m-1,k}(A, B) U$) is diagonal, then f

⁸Note, that the Schatten p -norm is actually defined [2] by

$$\left[\sum_{j=1}^n s_j(A)^p \right]^{\frac{1}{p}},$$

where $s_j(A)$, $j = 1, \dots, n$, are the singular values of A . For positive hermitian matrices, however, our notion coincides with that definition. As we are interested in the case of positivity only, we may sloppily re-use the notion p -“norm” for our case. In fact, our definition does not give a norm on the linear space of all $n \times n$ matrices.

⁹ Observe that

$$\|A e^{xC}\|_p'(0) = \frac{1}{p} \|A\|_p^{1-p} (\|A e^{xC}\|_p^p)'(0) = \frac{1}{p} \|A\|_p^{1-p} (\operatorname{tr} (A e^{xC})^p)'(0) = \|A\|_p^{1-p} \operatorname{tr} A^p C$$

and, therefore,

$$f'(0) = \frac{1}{\|A\|_p^2} (AC \|A\|_p - A \|A\|_p^{1-p} \operatorname{tr} A^p C) = \frac{1}{\|A\|_p^{p+1}} (AC \|A\|_p^p - A \operatorname{tr} A^p C).$$

is positive and hermitian for any $C = UDU^*$ with D being diagonal and real. In fact, the product of diagonal positive and hermitian matrices has these properties again. If now A and B are nonzero and again extremal for $\text{tr } S_{m,k}$ among n -phone matrices, then

$$\begin{aligned} 0 &= \frac{\|A\|_p^{p+1}}{m} \text{tr } S'_{m,k}(f, B)|_{x=0} = \text{tr}((AC \text{tr } A^p - A \text{tr } A^p C) S_{m-1,k}(A, B)) \\ &= \text{tr}(S_{m-1,k}(A, B) A \text{tr } A^p - A^p \text{tr } S_{m-1,k}(A, B) A) C. \end{aligned}$$

Since $S_{m-1,k}(A, B)$ and A commute as seen above and are hermitian, we get

$$S_{m-1,k}(A, B) A \text{tr } A^p = A^p \text{tr } S_{m-1,k}(A, B) A$$

from Lemma B.2. Similarly, we can derive

$$S_{m-1,k-1}(A, B) B \text{tr } B^p = B^p \text{tr } S_{m-1,k-1}(A, B) B.$$

Altogether we have

Proposition A.1 If $0 < k < m$ and if $\text{tr } S_{m,k}$ is extremal at (A, B) for the positive hermitian matrices having unit p -norm with $1 \leq p < \infty$, then

$$\begin{aligned} S_{m-1,k}(A, B) A &= A^p \text{tr } S_{m-1,k}(A, B) A \\ S_{m-1,k-1}(A, B) B &= B^p \text{tr } S_{m-1,k-1}(A, B) B. \end{aligned}$$

The case $p = 2$ has already been derived by Hillar in [6]. There, the norm equals the Frobenius norm. The case $p = \infty$, i.e., the supnorm case, can be dealt with as for $p < \infty$ as far as we derive that A and $S_{m-1,k}(A, B)$ commute. Assuming now, for simplicity, that A and $S_{m-1,k}(A, B)$ are diagonal and $\|A\| = 1$, we see that $f(x) := Ae^{xC}$ is (at least for small $|x|$) n -phone — provided C is diagonal with $C_{ii} = 0$ for $A_{ii} = 1$. Then $f'(0) = AC$ implying $\text{tr } ACS_{m-1,k}(A, B) = 0$, whence the (i, i) components of $S_{m-1,k}(A, B)A$ vanish if $A_{ii} \neq 1$. If P_A has a single nonzero entry, then we immediately get $S_{m-1,k}(A, B)A = P_A \text{tr } S_{m-1,k}(A, B)A$. In the other case, however, we run into the non-differentiability problem as above. At present, we are not able to solve this problem.

Nevertheless, we have

Corollary A.2 If $0 < k < m$ and if $\text{tr } S_{m,k}$ is extremal at (A, B) for the positive hermitian matrices having unit p -norm with $1 \leq p < \infty$, then

$$S_{m,k}(A, B) = \frac{(m-k)A^p + kB^p}{m} \text{tr } S_{m,k}(A, B).$$

The same is true for $p = \infty$, provided P_A and P_B have rank 1.

Proof Use

$$\begin{aligned} (m-k) \text{tr } S_{m,k}(A, B) &= m \text{tr } AS_{m-1,k}(A, B) \\ k \text{tr } S_{m,k}(A, B) &= m \text{tr } BS_{m-1,k-1}(A, B) \end{aligned}$$

(for a proof see Lemma 2.1 in [6]) and

$$S_{m,k}(A, B) = AS_{m-1,k}(A, B) + BS_{m-1,k-1}(A, B).$$

qed

B Lie Algebra Relations

Lemma B.1 If A and S are hermitian matrices, fulfilling $\text{tr } [A, C]S = 0$ for all $C \in \mathfrak{su}(n)$, then A and S commute.

Proof Since A and S are hermitian, we have $[A, S]^* = -[A, S]$ and, anyway, $\text{tr}[A, S] = 0$. Therefore, $[A, S] \in \mathfrak{su}(n)$. Moreover, $\text{tr}[S, A]C = \text{tr}[A, C]S$ vanishes by assumption for any $C \in \mathfrak{su}(n)$. Since $\mathfrak{su}(n)$ is semisimple, the Killing form $(X, Y) := \frac{1}{n} \text{tr}(XY)$ on $\mathfrak{su}(n)$ is non-degenerate, giving $[S, A] = \mathbf{0}$. **qed**

Lemma B.2 If A and S are hermitian matrices that are diagonal after conjugation with U and fulfill $\text{tr}((SA \text{tr} A^L - A^L \text{tr} SA)UDU^*) = 0$ for all diagonal matrices D , then $SA \text{tr} A^L = A^L \text{tr} SA$.

Proof If A and S are already diagonal, then the assertion is trivial. In fact, letting D be the matrix having just a single nonzero entry at position (i, i) , the trace equation above means that the (i, i) component of $(SA \text{tr} A^L - A^L \text{tr} SA)$ vanishes. Since the off-diagonal elements are zero anyway, we get the assertion.

In the general case observe that

$$\begin{aligned} \text{tr}(U^* S U U^* A U \text{tr}(U^* A U)^L - (U^* A U)^L \text{tr} U^* S U U^* A U) D \\ = \text{tr}(SA \text{tr} A^L - A^L \text{tr} SA)UDU^* \end{aligned}$$

reduces this case to the first one. **qed**

C Simple, But Useful Identity

Lemma C.1 For any $n \times n$ matrices X_i and X , we have

$$X_1 \cdots X_k = X^k + \sum_{i=1}^k X^{i-1} (X_i - X) X_{i+1} \cdots X_k.$$

Proof For $k = 1$, we have $X_1 = X^1 + X^0 (X_1 - X)$. For $k > 1$, we have by induction

$$\begin{aligned} X_1 \cdots X_{k+1} &= X^k X_{k+1} + \sum_{i=1}^k X^{i-1} (X_i - X) X_{i+1} \cdots X_k X_{k+1} \\ &= X^k (X + (X_{k+1} - X)) + \sum_{i=1}^k X^{i-1} (X_i - X) X_{i+1} \cdots X_k X_{k+1} \\ &= X^k X + \sum_{i=1}^{k+1} X^{i-1} (X_i - X) X_{i+1} \cdots X_k X_{k+1}. \end{aligned}$$

qed

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